

Majorana fermions in density modulated p-wave superconducting wires

Li-Jun Lang¹ and Shu Chen^{1,*}

¹*Beijing National Laboratory for Condensed Matter Physics,
Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

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We study the p-wave superconducting wire with a periodically modulated chemical potential and show that the Majorana edge states are robust against the modulation of density. In some particular regimes, the Majorana fermions are greatly enhanced by the periodic modulation. The existence of Majorana edge fermions in the open chain can be characterized by a topological Z_2 invariant of the bulk system, which can be applied to determine the phase boundary between the topologically trivial and nontrivial superconducting phases. We also demonstrate the existence of the zero-energy peak in the spectral function of the topological superconducting phase, which is only sensitive to the open boundary condition but robust against the disorder.

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Introduction.— Searching for Majorana fermions (MFs) in condensed matter systems has attracted intensive studies in past years [1, 2], due to the fundamental interest in exploring the new type of particles fulfilling non-Abelian statistics and the potential applications for the topological quantum computing [1–6]. Among various proposals for realizing the emergent MFs, the quantum wires with p-wave pairings provide promising candidates for realizing emergent MFs at the ends of wires. As shown in the original work of Kitaev [3], boundary MFs emerge in the one-dimensional (1D) p-wave superconductor if the system is in a topological phase. Moreover, quantum wires with a strong spin-orbit coupling, or topologically insulating wires, subject to a Zeeman magnetic field and in proximity of a superconductor, are found to exhibit boundary MFs [7, 8]. Particularly, experimental signatures of MFs in hybrid superconductor-semiconductor nanowires have been reported very recently [9], which stimulates the study of exploring MFs in 1D systems [10–16]. Schemes of realizing Majorana chains have also been proposed in cold atomic systems [17], carbon nanotubes [18], superconducting (SC) circuits [19] and quantum-dot-superconductor arrays [20].

As most of theoretical works focus on ideal homogeneous wires with a uniform chemical potential, an important problem is the stability of the MFs under the modulation of density and disorder. In this work, we explore the nonuniform p-wave SC wires with a periodic modulation of the chemical potential, extending the Kitaev’s p-wave SC model [3], and study the fate of the MFs under the density modulation and disorder. In general, a periodically modulated potential is of benefit to the formation of periodic density waves. If the modulation amplitude is large, one may expect that the SC phase could be destroyed. As the robustness of Majorana mode is protected by the SC gap, the MFs may be unstable in the presence of density modulation and disorder. On the other hand, recent work on the density modulated wires in the absence of SC order parameter indicates the exis-

tence of topologically protected edge states [21, 22]. So far, it is unclear whether the Majorana edge states is enhanced or suppressed under the density modulation. The current work will focus on this problem and show the robustness of Majorana edge states against the density modulation and disorder. Particularly, in some parameter regimes, we find that MFs always exist for the arbitrarily strong modulation strength, which may shed light on the design of quantum architectures producing robust MFs.

Model of density modulated p-wave superconductors.— We consider a typical lattice model of the 1D p-wave superconductor with modulated chemical potentials, which is described by

$$H = \sum_i [(-tc_i^\dagger c_{i+1} + \Delta c_i c_{i+1} + H.c.) - \mu_i c_i^\dagger c_i], \quad (1)$$

where \hat{c}_i^\dagger (\hat{c}_i) is the creation (annihilation) operator of fermions at the i -th site, t the nearest-neighbor hopping amplitude, Δ the p-wave SC order parameter and chosen real, and the modulated chemical potential given by

$$\mu_i = V \cos(2\pi i\alpha + \delta) \quad (2)$$

with V being the strength, $\alpha = p/q$ a rational number (p and q are co-prime integers), and δ an arbitrary phase. The modulated chemical potential can be generated by the bichromatic optical lattice for cold atom systems [17, 23] or through the control of gates for quantum-dot arrays and quantum wires [20, 24].

In order to diagonalize the quadratic form Hamiltonian, we resort to the Bogoliubov-de Gennes transformation [25, 26] and define a set of new fermionic operators,

$$\eta_n^\dagger = \frac{1}{2} \sum_{i=1}^L [(\phi_{n,i} + \psi_{n,i})c_i^\dagger + (\phi_{n,i} - \psi_{n,i})c_i], \quad (3)$$

where L is the number of lattice sites and $n = 1, \dots, L$. For convenience, $\phi_{n,i}$ and $\psi_{n,i}$ are chosen to be real due

to the reality of all the coefficients in the Hamiltonian (1). In terms of the operators η_n and η_n^\dagger , the Hamiltonian (1) is diagonalized as $H = \sum_{n=1}^L \Lambda_n (\eta_n^\dagger \eta_n - \frac{1}{2})$, where Λ_n is the spectrum of the single quasi-particles. From the diagonalization condition, $[\eta_n, H] = \Lambda_n \eta_n$, we can get the following coupled equations:

$$\begin{aligned}\Lambda_n \phi_{n,i} &= (\Delta - t) \psi_{n,i+1} - \mu_i \psi_{n,i} - (\Delta + t) \psi_{n,i-1}, \\ \Lambda_n \psi_{n,i} &= -(\Delta + t) \phi_{n,i+1} - \mu_i \phi_{n,i} + (\Delta - t) \phi_{n,i-1},\end{aligned}\quad (4)$$

with $i = 1, \dots, L$. From Eqs. (4), one can prove that if the equations have the solution of $(\phi_{n,i}, \psi_{n,i})$ ($i = 1, \dots, L$) with a positive eigenvalue $\Lambda_n > 0$, $(\phi_{n,i}, -\psi_{n,i})$ is also the solution with the eigenvalue $-\Lambda_n$, which implies $\eta_n(\Lambda_n) = \eta_n^\dagger(-\Lambda_n)$.

Boundary Majorana fermions.- The solution to Eqs. (4) is related to the boundary condition. The boundary Majorana states can only exist in the system with open boundary conditions (OBC). To seek such a state, we solve Eqs. (4) under OBC of $\psi_{n,L+1} = \psi_{n,0} = \phi_{n,L+1} = \phi_{n,0} = 0$, and the Majorana edge states correspond to the zero mode solution of $\Lambda_n = 0$. For $\Lambda_n = 0$, ϕ_i and ψ_i are decoupled and Eqs. (4) can be written in the transfer matrix form

$$\begin{aligned}(\phi_{n,i+1}, \phi_{n,i})^T &= A_i(\phi_{n,i}, \phi_{n,i-1})^T, \\ (\psi_{n,i-1}, \psi_{n,i})^T &= A_i(\psi_{n,i}, \psi_{n,i+1})^T,\end{aligned}\quad (5)$$

with $A_i = \begin{pmatrix} \frac{-\mu_i}{\Delta+t} & \frac{\Delta-t}{\Delta+t} \\ 1 & 0 \end{pmatrix}$. To understand the boundary Majorana mode, we rewrite the operators (3) as

$$\eta_n^\dagger = \frac{1}{2} \sum_{i=1}^L [\phi_{n,i} \gamma_i^A + i \psi_{n,i} \gamma_i^B], \quad (6)$$

where $\gamma_i^A = c_i^\dagger + c_i$ and $\gamma_i^B = i(c_i - c_i^\dagger)$ are operators of two MFs, which fulfill the relations $(\gamma_i^\alpha)^\dagger = \gamma_i^\alpha$ and $\{\gamma_i^\alpha, \gamma_j^\beta\} = 2\delta_{ij}\delta_{\alpha\beta}$ with α and β taking A or B . Coefficients of $\phi_{n,i}$ and $\psi_{n,i}$ in Eq. (3) are just the amplitudes of Majorana operators γ_i^A and γ_i^B , respectively. If there exists a zero mode solution, according to Eqs. (5), we will get a decaying solution for one set of coefficients and a growing one for the other. An example is the special case with $V = 0$ and $\Delta = t$ [3], for which the zero mode solution is given by $(\phi_1, \phi_2, \dots, \phi_L) = (1, 0, \dots, 0)$ and $(\psi_1, \dots, \psi_{L-1}, \psi_L) = (0, \dots, 0, 1)$. In this case, $\eta^\dagger(\Lambda = 0) = \frac{1}{2}[\gamma_1^A + i\gamma_L^B]$, which means that the zero mode state is divided into two separated MFs located at the left and right ends, respectively.

For the commensurate potential with $\alpha = p/q$, A_i is q -periodic. One can judge whether the zero mode solution exists by evaluating the two eigenvalues of the product matrix $A = \prod_{i=1}^q A_i$ [15]. If both of them are either smaller or greater than unity, there is a zero mode solution with MFs located at the ends, otherwise no zero

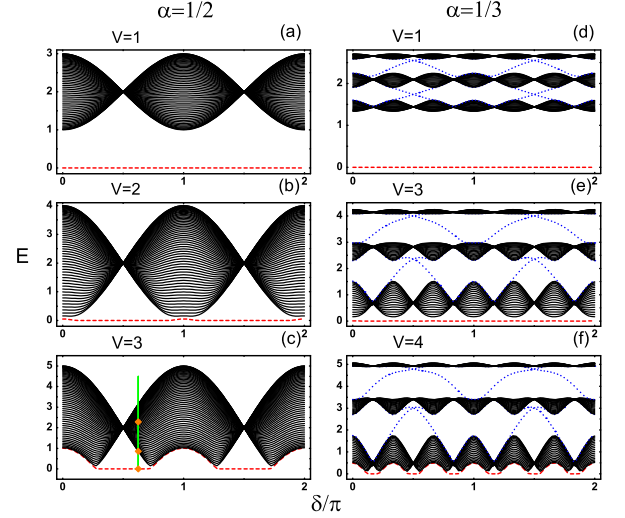


FIG. 1: The energy spectra of 1D modulated p-wave superconductors vs the phase factor, δ , under OBC for $\alpha = \frac{1}{2}$ ((a)-(c)) and $\frac{1}{3}$ ((d)-(f)). The red dashed lines are the lowest excitation states and the blue dotted ones are the edge states in the excitation gaps. These figures are calculated with parameters $t = \Delta = 1$ and $L = 101$.

mode solution is available. Solving Eqs. (4), we can get the whole excitation spectrum for the single quasi-particles. In Fig.1, we show the spectra for cases of $\alpha = 1/2$ and $1/3$ under OPC. It is shown that the zero mode solutions exist in the whole phase parameter space when V is smaller than a critical value. When V exceeds a critical value, the regimes for the existence of the zero mode solutions in the phase parameter space become narrow. However, our numerical results indicate that the zero mode Majorana solutions *always* exist at some specific values of δ , no matter how strong the strength V is. For the systems with $\alpha = 1/2$ and $1/3$ shown in Fig.1, the specific values of δ are $\frac{(2m+1)\pi}{2}$ for $\alpha = 1/2$ and $\frac{(2m+1)\pi}{6}$ for $\alpha = 1/3$ with m being an integer. At these specific values δ_s , the critical value of the phase transition, $V_c(\Delta, \delta_s)$, which is a function of Δ and δ , tends to infinity. When deviated from these points, there exists a finite critical value, $V_c(\Delta, \delta)$, above which there appears a topologically trivial phase without zero mode MFs.

In order to see clearly the differences between the zero mode state and nonzero mode states, we display distributions of ϕ_i and ψ_i for the zero mode solution and solutions with nonzero eigenvalues of quasi-particles located at the bottom and center of the continuous band (orange squares along the green cut in Fig. 1(c)). As shown in Fig.2, for the system with $\delta = 5\pi/8$ and $V = 3$, the amplitudes of the Majorana operators for the zero mode solution are located at the left and right ends, respectively. As ϕ_i (ψ_i) decays very quickly away from the left (right) edge, there is no overlap for the Majorana modes of γ_i^A and γ_i^B . As a comparison, distributions of ϕ_i and

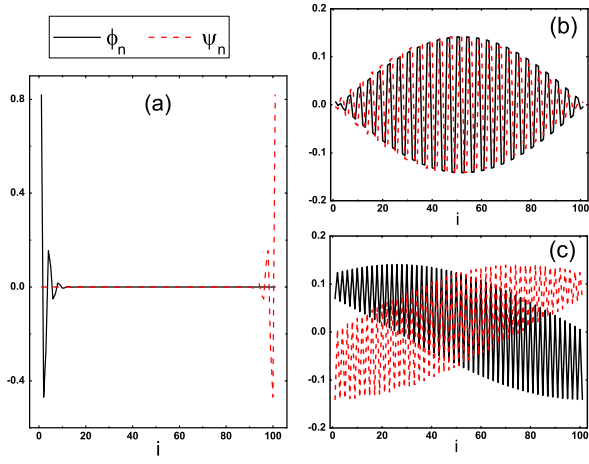


FIG. 2: The amplitudes of ϕ_n (black solid) and ψ_n (red dashed), for excitation states labelled by orange squares along the green cut in Fig. 1(c). From bottom to top, (a), (b), and (c) represent the states of zero mode, at the bottom and at the center of the bulk band, respectively. They are calculated with parameters $V = 3$, $\alpha = \frac{1}{2}$, $t = \Delta = 1$, $\delta = \frac{5\pi}{8}$ and $L = 101$ under OBC.

ψ_i for nonzero modes spread over the whole regime and the corresponding quasiparticle operator can not be split into two separated Majorana operators.

Z_2 topological invariant.— The presence or absence of zero mode MFs is determined by the Z_2 topological class of the bulk superconductor. As no boundary zero mode solution is available for the system with periodic boundary conditions (PBC), we can choose a Z_2 topological invariant (or ‘Majorana number’) [3] to characterize the topological nature of the bulk system. In order to define such a topological invariant, we shall consider the system with PBC. For the periodic system with $\alpha = p/q$, it is convenient to use the Fourier transform, $c_i = c_{s,l} = \sqrt{\frac{q}{L}} \sum_k c_{s,k} e^{ikql}$ with $i = s + (l-1)q$, which transforms the Hamiltonian (1) into $H = \sum_k [\sum_{s=1}^{q-1} (-tc_{s,k}^\dagger c_{s+1,k} + \Delta c_{s,k} c_{s+1,-k}) - tc_{q,k}^\dagger c_{1,k} e^{ikq} + \Delta c_{q,k} c_{1,-k} e^{-ikq} + H.c.] - \sum_k \sum_{s=1}^q \mu_s (c_{s,k}^\dagger c_{s,k} - \frac{1}{2})$, where $s = 1, \dots, q$ is the index of inner sites in a supercell, $l = 1, \dots, L/q$ the index of the l -th supercell, and k the momentum defined in the reduced Brillouin zone of $[0, 2\pi/q)$. Then we define a set of new operators [12]:

$$\gamma_{2s-1}(k) = c_{s,k} + c_{s,-k}^\dagger, \quad \gamma_{2s}(k) = (c_{s,k} - c_{s,-k}^\dagger)/i, \quad (7)$$

with the anticommutation relations $\{\gamma_m^\dagger(k), \gamma_n(k')\} = 2\delta_{mn}\delta_{kk'}$ and $\gamma_m^\dagger(k) = \gamma_m(-k)$. $\gamma_m(0)$ and $\gamma_m(\pi/q)$ are just Majorana operators due to $\gamma_m^\dagger(0) = \gamma_m(0)$ and $\gamma_m^\dagger(\pi/q) = \gamma_m(-\pi/q) = \gamma_m(\pi/q)$. In the basis of the new operators, we can transform the Hamiltonian into the form:

$$H = \frac{i}{4} \sum_k \sum_{m,n} B_{m,n}(k) \gamma_m(-k) \gamma_n(k), \quad (8)$$

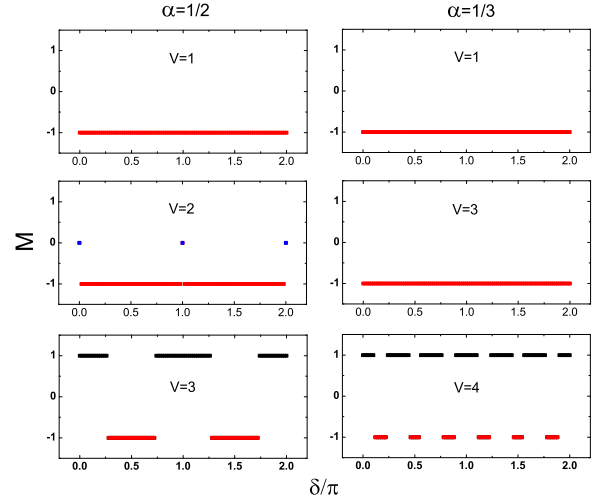


FIG. 3: Z_2 topological invariant, M , vs the phase factor, δ , for system with $t = \Delta = 1$, $\alpha = \frac{1}{2}$ ((a)-(c)) and $\frac{1}{3}$ ((d)-(f)) under PBC.

with $B_{2s-1,2s}(k) = -B_{2s,2s-1}(k) = -\mu_s$ for $s = 1, \dots, q$, $B_{2s-1,2s+2}(k) = -B_{2s+2,2s-1}(k) = \Delta - t$, $B_{2s,2s+1}(k) = -B_{2s+1,2s}(k) = \Delta + t$ for $s = 1, \dots, q-1$, $B_{1,2q}(k) = -B_{2q,1}^*(k) = -(\Delta + t)e^{-ikq}$, and $B_{2,2q-1}(k) = -B_{2q-1,2}^*(k) = -(\Delta - t)e^{-ikq}$.

The parameters $B_{m,n}(k)$ form a $2q \times 2q$ matrix $B(k)$, and here only $B(0)$ and $B(\pi/q)$ are skew-symmetric. Following Kitaev [3, 12], we can calculate the Z_2 topological invariant defined as:

$$M = \text{sgn}[\text{Pf}(B(0))]\text{sgn}[\text{Pf}(B(\pi/q))], \quad (9)$$

where $\text{Pf}(X) = \frac{1}{2^N N!} \sum_P \text{sgn}(P) X_{P_1 P_2} \cdots X_{P_{2N-1} P_{2N}}$ is the Pfaffian of the skew-symmetric matrix X with P standing for a permutation of $2N$ elements of X and $\text{sgn}(P)$ the corresponding sign of the permutation. According to the definition, generally we have $M = \pm 1$ with $M = 1$ corresponding to a Z_2 -topologically trivial phase and $M = -1$ to a Z_2 -topologically non-trivial phase. In Fig.3, we display the Z_2 topological invariant versus the phase factor δ for systems with the same parameters as in Fig. 1. Comparing Fig.3 with Fig.1, we see the exact correspondence between the presence (absence) of zero mode MFs and -1 ($+1$) value of the Z_2 topological invariant. Especially, M takes the value of 0 (blue square dots in Fig.3(b)) at $V = 2$, which is just the critical point V_c of the phase transition from a Z_2 -topologically non-trivial phase to a topologically trivial phase for the corresponding δ . In principle, we can always determine $V_c(\Delta, \delta)$ through the condition of $M = 0$ and give the whole phase diagram.

Phase diagram.— Without loss of generality, we choose $\Delta, V \geq 0$ in the following discussion. From the definition of the matrix $B(k)$, we know that for $\alpha = 1/2$, $\text{Pf}[B(0)] = -V^2 \cos^2 \delta - 4t^2$ and $\text{Pf}[B(\pi/2)] =$

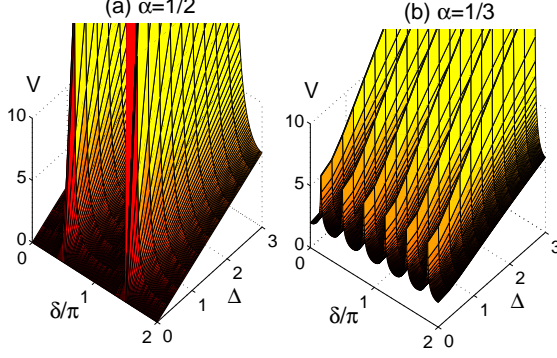


FIG. 4: Phase diagrams expanded by V , Δ , and δ for the cases of (a) $\alpha = 1/2$ and (b) $\alpha = 1/3$. The curved surfaces are the phase boundaries above which is Z_2 -topologically trivial while below which is Z_2 -topologically non-trivial.

$-V^2 \cos^2 \delta + 4\Delta^2$. Here due to $\text{Pf}[B(0)] < 0$, we just need to set $\text{Pf}[B(\pi/2)] = 0$ to get the phase boundary condition, that is, $V^2 \cos^2 \delta = 4\Delta^2$, or equivalently $V|\cos \delta| = 2\Delta$ (Fig. 4(a)). Likewise, for $\alpha = 1/3$, $\text{Pf}[B(0)] = -\frac{V^3}{4} \cos 3\delta - 2t(t^2 + 3\Delta^2)$ and $\text{Pf}[B(\pi/3)] = -\frac{V^3}{4} \cos 3\delta + 2t(t^2 + 3\Delta^2)$. The phase boundary condition can be also got easily as $V^3|\cos 3\delta| = 8t(t^2 + 3\Delta^2)$ (Fig. 4(b)). From Fig. 4, we see clearly again that there exist some specific points δ_s , at which the system is always Z_2 -topologically non-trivial for arbitrary V . On the other hand, the critical value, $V_c(\Delta, \delta)$, increases with the increase of the SC pairing amplitude Δ .

For the general case of $\alpha = p/q$, we can infer the phase boundary condition by analyzing the expression of Pfaffian. The non-permuted term, $B_{12}B_{34}\cdots B_{2q-1,2q}$, gives $(-1)^q \prod_{s=1}^q \mu_s$. Due to the sparsity of the matrix B , we see that there are only three kinds of permutations which contribute non-zero terms: 1. $B_{2s-1,2s}B_{2s+1,2s+2} \rightarrow B_{2s-1,2s+2}B_{2s,2s+1}$ or $B_{1,2}B_{2q-1,2q} \rightarrow B_{1,2q}B_{2,2q-1}$, which makes a replacement of $\mu_s\mu_{s+1}$ or $\mu_1\mu_q$ in the non-permuted term by $(\Delta^2 - t^2)$ or $(\Delta^2 - t^2)e^{-2ikq}$, respectively; 2. $B_{2s-1,2s} \rightarrow B_{2s,2s+1}$ ($s = 1, \dots, q-1$) and $B_{2q-1,2q} \rightarrow B_{1,2q}$, which gives $-(t + \Delta)^q e^{-ikq}$; 3. $B_{2s-1,2s} \rightarrow B_{2s-1,2s+2}$ ($s = 1, \dots, q-1$) and $B_{2q-1,2q} \rightarrow B_{2,2q-1}$, which gives $-(t - \Delta)^q e^{-ikq}$. These permutations are independent of each other. Our numerical study shows that when $k = 0$ and π/q , the sum of all terms generated by the first kind of permutations is zero except the full-permuted ones (if there is) without any $-\mu_s$ left. So the first kind contributes a term of 0 for odd q 's or $(\Delta^2 - t^2)^{q/2} + (\Delta^2 - t^2)^{q/2} e^{-2ikq}$ for even q 's. Thus we have $\text{Pf}[B(0)] = -\prod_{s=1}^q \mu_s - [(t + \Delta)^q + (t - \Delta)^q]$ for odd q 's or $\prod_{s=1}^q \mu_s - [(t + \Delta)^{q/2} - (-1)^{q/2}(t - \Delta)^{q/2}]^2$ for even q 's, and $\text{Pf}[B(\pi/q)] = -\prod_{s=1}^q \mu_s + [(t + \Delta)^q + (t - \Delta)^q]$ for odd q 's or $\prod_{s=1}^q \mu_s + [(t + \Delta)^{q/2} + (-1)^{q/2}(t - \Delta)^{q/2}]^2$ for

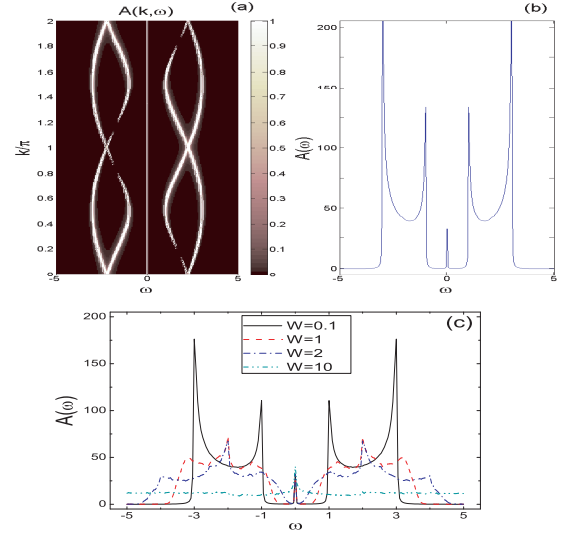


FIG. 5: The spectral functions and the disorder effects. Here, as example, we choose $\alpha = 1/2$, $\delta = 0$ to plot (a) the momentum-resolved spectral function, $A(k, \omega)$, and (b) the corresponding total spectral function, $A(\omega)$, without disorder, i.e. $W = 0$. (c) shows that the total spectral function, $A(\omega)$, varies with the strength of disorder. The other parameters are $L = 250, t = \Delta = V = 1$ under OBC. We have done 500 realizations to calculate the disorder effects.

even q 's. Therefore, we can get the general formula for the boundaries: $|\prod_{s=1}^q \mu_s| = (t + \Delta)^q + (t - \Delta)^q$ for odd q 's, and $-\prod_{s=1}^q \mu_s = (t + \Delta)^q + (t - \Delta)^q + 2(\Delta^2 - t^2)^{q/2}$ ($\prod_{s=1}^q \mu_s < 0$) or $\prod_{s=1}^q \mu_s = (t + \Delta)^q + (t - \Delta)^q - 2(\Delta^2 - t^2)^{q/2}$ ($\prod_{s=1}^q \mu_s > 0$) for even q 's. The special cases of $\alpha = 1/2$ and $1/3$ can be derived from these general formula.

Spectral function.— As the Majorana edge states correspond to the zero mode solution protected by the presence of an energy gap, one would expect a zero-energy peak appearing in the corresponding spectral function. The momentum-resolved spectral function with momentum k and energy ω ($\hbar = 1$) is defined as $A(k, \omega) = -\frac{1}{\pi} \text{Im} G_r(k, \omega)$, where $G_r(k, \omega) = \int_{-\infty}^{\infty} G_r(k, t) e^{i\omega t - 0^+ t} dt$ and $G_r(k, t) = -i\theta(t) \langle G | \{c_k(t), c_k^\dagger(0)\} | G \rangle$ is the single particle (retarded) Green function with $|G\rangle$ being the ground state of the system, and $c_k(t) = e^{iHt} c_k e^{-iHt}$ is the fermionic annihilation operator in the moment space with $c_k = \frac{1}{\sqrt{L}} \sum_j c_j e^{-ikj}$. And the corresponding total spectral function is $A(\omega) = \sum_k A(k, \omega)$. As shown in Fig.5(a) and (b), an obvious zero-energy peak is observed for the system with OBC. On the contrary, we find no zero-energy peak in the system with PBC.

The Majorana edge states are expected to be immune to local perturbations. To explore the effect of disorder, here we add a random on-site potential, $H_D = \sum_i W_i c_i^\dagger c_i$, to the Hamiltonian (1), which usually leads to Anderson localizations, where W_i is uniformly distributed in the range of $[-W/2, W/2]$ with W being the

disorder strength. Fig. 5(c) shows that even though the energy gaps between the zero mode and the excitation modes are smeared by disorder, the zero-energy peak is still notable, although it is becoming shorter as well. It again indicates that the MFs appearing in our system are robust against local perturbations as expected.

Summary.- In summary, we find that in the density modulated p-wave SC wires, by tuning the phase parameter, the zero mode Majorana edge states emerge in some intervals, and some of them are strong enough, independent of the strength of the periodic density modulation. The appearance of the MFs demonstrate the Z_2 topological nature. After calculating the Z_2 topological invariant, we get the phase diagram for the transition from topologically nontrivial phases to trivial phases. By this model, we supply a good platform to have possible schemes of searching for MFs. At last, we also give an evidence in the spectral function where a zero-energy peak appears under OBC, even subject to strong disorder. The spectral function is possible to be experimentally detected by the photoemission spectroscopy.

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* Electronic address: schen@aphy.iphy.ac.cn

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